

Propranolol bis(trifluoroacetate)

Other names:	Propranolol, bis-TFA propranolol, TFA
Inchi:	InChI=1S/C20H19F6NO4/c1-12(2)27(17(28)19(21,22)23)10-14(31-18(29)20(24,25)26)11
InchiKey:	QALUHRIUDJFKPS-UHFFFAOYSA-N
Formula:	C20H19F6NO4
SMILES:	CC(C)N(CC(COc1cccc2ccccc12)OC(=O)C(F)(F)F)C(=O)C(F)(F)F
Mol. weight [g/mol]:	451.36
CAS:	40435-87-8

Physical Properties

Property code	Value	Unit	Source
gf	-1198.17	kJ/mol	Joback Method
hf	-1666.79	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.492		Crippen Method
mvol	284.920	ml/mol	McGowan Method
pc	1368.70	kPa	Joback Method
tb	860.94	K	Joback Method
tc	1061.72	K	Joback Method
tf	541.97	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.73	J/molxK	860.94	Joback Method
cpg	904.28	J/molxK	894.40	Joback Method
cpg	915.91	J/molxK	927.87	Joback Method
cpg	926.72	J/molxK	961.33	Joback Method
cpg	936.79	J/molxK	994.79	Joback Method
cpg	946.22	J/molxK	1028.26	Joback Method
cpg	955.09	J/molxK	1061.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40435878&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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